

**HIGH PRODUCTION VOLUME (HPV)
CHALLENGE PROGRAM**

TEST PLAN

For

1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio)

**Prepared by
The American Chemistry Council
Petroleum Additives Panel
Health, Environmental, and Regulatory Task Group**

August 13, 2003

**LIST OF MEMBER COMPANIES IN THE
HEALTH, ENVIRONMENTAL AND REGULATORY TASK GROUP**

The Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council Petroleum Additives Panel includes the following member companies:

BP plc

Chevron Oronite Company, LLC

Crompton Corporation

Ethyl Corporation

ExxonMobil Chemical Company

Ferro Corporation

Infineum

The Lubrizol Corporation

Rhein Chemie Corporation

Rhodia, Inc. (formerly Albright & Wilson Americas Inc.)

1.0 INTRODUCTION

In March 1999, the American Chemistry Council (formerly the Chemical Manufacturers Association) Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG), and its participating member companies committed to address data needs for certain chemicals listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. This test plan follows up on that commitment. Specifically, this test plan sets forth how the HERTG intends to address testing information for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio), CAS Number: 89347-09-1.

In preparing this test plan the following steps were undertaken:

Step 1: A review of the literature and confidential company data was conducted on the physicochemical properties, mammalian toxicity endpoints, and environmental fate and effects for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio), using its CAS number, CAS name, and synonyms. Searches included the following sources: MEDLINE, BIOSIS, CANCERLIT, CAPLUS, CHEMLIST, EMBASE, HSDB, RTECS, EMIC, and TOXLINE databases; the TSCATS database for relevant unpublished studies on these chemicals; and standard handbooks and databases (e.g., Sax, CRC Handbook on Chemicals, IUCLID, Merck Index, and other references) for physicochemical properties.

Step 2: The compiled data was evaluated for adequacy in accordance with the EPA guidance documentation.

2.0 GENERAL SUBSTANCE INFORMATION

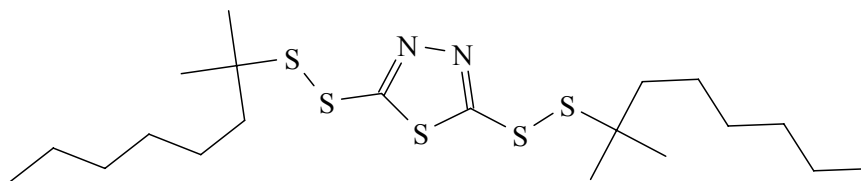
Chemical Name: 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio)

Chemical Abstract Service Registry Number: CAS No.: 89347-09-1

Molecular Formula: C₂₀H₃₈N₂S₃

Molecular Weight: 466.84 g/mol

Structural Diagram:



1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio)

3.0 USE, MANUFACTURE, DISTRIBUTION AND EXPOSURE INFORMATION

3.1 Use Information

1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio) is used to formulate finished greases and lubricating oils including industrial, gear, automatic transmission and some types of automotive crankcase, heavy duty diesel and medium speed diesel oils. In these applications, it is used as an ashless copper corrosion inhibitor and extreme pressure (EP) agent.

In lubricant applications, 1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio) is generally used in dosages starting at 0.01 wt.% for industrial oils and ranging from 0.045 wt.% to 0.15% in automotive oils depending on the type of basestock. To obtain extreme pressure properties, treat levels are generally in the range of 0.15 to 0.30 wt. %.

1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio) is also used as a sulfur deactivator, corrosion inhibitor and antioxidant in gasoline, heating oil and Liquified Petroleum Gas. However, its use in these applications is very limited. Fuel treatment levels are in the range of 10 - 100 PPM depending upon the active sulfur level of the fuel.

1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio) is generally sold to fuel blenders in its neat form, while finished oil blenders receive this component in both its neat form and in additive packages, where the concentration typically ranges from 0.3 to 3.5 wt.%. These additive packages are then blended into finished oils where the typical concentration of 1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio) ranges from 0.01 to 0.30 wt.% in the finished oil.

3.2 Manufacture, Distribution and Exposure Information

1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio) is manufactured and blended into additive packages at plants owned by members of the HERTG. As manufactured, this additive component

contains 80 - 90 wt.% 1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio) and 10 - 20 wt.% residual 2-Mercapto-5-tert-nonyldithio-1,3,4-thiadiazole. The 10 – 20 wt.% 2-Mercapto-5-tert-nonyldithio-1,3,4-thiadiazole in the additive component is residual from the manufacturing process and is not isolated during the life cycle of the additive component. Finished lubricants are blended at facilities owned by HERTG customers. The neat component is shipped in 55-gallon steel drums while additive packages containing this component are shipped to customers in bulk in ships, isocontainers, railroad tank cars, tank trucks or in 55-gallon steel drums. The bulk additive packages are stored in bulk storage tanks at the customer blending sites. Finished oils are blended by pumping the lubricating oil blend stocks and the additive package from their storage tanks through computer controlled valves that meter the precise delivery of the components into a blending tank. After blending, the finished lubricant products are sold in bulk and shipped in tank trucks to large industrial users, such as manufacturing facilities and facilities that service truck fleets and passenger motor vehicles. Finished lubricants are also packaged into 55-gallon drums, 5-gallon pails, and one-gallon and one-quart containers for sale to smaller industrial users. Sales of lubricants in one-gallon and one-quart containers to consumers at service stations or retail specialty stores also occur.

Based on these uses, the potentially exposed populations include (1) workers involved in the manufacture of 1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio), blending them into additive packages or fuels, and blending the additive packages into finished lubricants; (2) quality assurance workers who sample and analyze these products to ensure that they meet specifications; (3) workers involved in the transfer and transport of 1,3,4-Thiadiazole, 2,5-bis(tert-nonyldithio), additive packages or finished lubricants that contain them; (4) mechanics who may come into contact with both fresh and used lubricants while working on engines or equipment; (5) gasoline station attendants and consumers who may periodically add lubricating oil to automotive crankcases; and (6) consumers who may change their own automotive engine oil. The most likely route of exposure for these substances is skin and eye contact. Manufacturing, quality assurance, and transportation workers will likely have access to engineering controls and wear protective clothing to eliminate exposure. The most likely source of environmental exposure is accidental spills at manufacturing sites and during transport.

TABLE 1
SUMMARY TABLE OF AVAILABLE DATA

CAS No.: 89347-09-1	Study Date	Study Results	Data Acceptable
Physical/Chemical Characteristics			
<i>Melting Point</i>		Not Applicable	-
<i>Boiling Point</i>		No Data Located	-
<i>Vapor Pressure</i>		No Data Located	-
<i>Partition Coefficient</i>	1990	1.72-2.94 at 21° C	Yes
<i>Water Solubility</i>		No Data Located	-
Environmental Fate			
<i>Photodegradation</i>		No Data Located	-
<i>Hydrolysis</i>		No Data Located	-
<i>Fugacity</i>		No Data Located	-
<i>Biodegradation</i>	1989	<10% at 28 days	Yes
Ecotoxicity			
<i>Acute Toxicity to Algae</i>		No Data Located	-
<i>Acute Toxicity to Invertebrates</i>		No Data Located	-
<i>Acute Toxicity to Fish</i>	1985	96 Hr LC ₅₀ > 1000 mg/L 96 Hr NOEL = 1000 mg/L	Yes
Mammalian Toxicity			
<i>Acute Toxicity</i>	1981 1981 1981	Rat Oral LD ₅₀ >10 g/kg Rabbit Dermal LD ₅₀ > 2 g/kg Rat Inhalation LC ₅₀ > 2.75 mg/L	Yes Yes Yes
<i>Repeat Dose Toxicity</i>		No Data Located	-
<i>Developmental Toxicity</i>		No Data Located	-
<i>Reproductive Toxicity</i>		No Data Located	-
Genetic Toxicity			
<i>Gene Mutation</i>	1989	Not Mutagenic	Yes
<i>Chromosomal Aberration</i>	1989	Not Clastogenic	Yes

TABLE 2

SUMMARY TABLE OF PROPOSED TESTING

Based on the data availability indicated in the above “Summary Table of Available Data” the following HPV Testing is proposed:

CAS No.: 89347-09-1	Testing Required	OECD Test Guideline or Testing Model Proposed
Physical/Chemical Characteristics		
<i>Melting Point</i>	Not Applicable	
<i>Boiling Point</i>	Yes	OECD 102/103
<i>Vapor Pressure</i>	Yes	OECD 104
<i>Partition Coefficient</i>	No	-
<i>Water Solubility</i>	Yes	OECD 105
Environmental Fate		
<i>Photodegradation</i>	Yes	AOPWIN Model
<i>Hydrolysis</i>	Yes	Technical Discussion
<i>Fugacity</i>	Yes	Fugacity Level 1 Type Model
<i>Biodegradation</i>	No	-
Ecotoxicity		
<i>Acute Toxicity to Algae</i>	Yes	OECD 201
<i>Acute Toxicity to Invertebrates</i>	Yes	OECD 202
<i>Acute Toxicity to Fish</i>	No	-
Mammalian Toxicity		
<i>Acute Toxicity</i>	No	-
<i>Repeat Dose Toxicity</i>	Yes	OECD 422
<i>Developmental Toxicity</i>	Yes	OECD 422
<i>Reproductive Toxicity</i>	Yes	OECD 422
Genetic Toxicity		
<i>Gene Mutation</i>	No	-
<i>Chromosomal Aberration</i>	No	-

4.0 PHYSICAL CHEMICAL PROPERTIES

4.1.1 Summary of Available Data

The octanol/water partition coefficient of 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio) determined according to OECD Guideline 107 is 1.72-2.94 at 21° C.

4.1.2 Data Assessment and Test Plan for Physicochemical Properties Relevant to Environmental Fate

Adequate and reliable octanol/water partition coefficient data is available for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio). No published or unpublished data were located in a literature search for melting point, boiling point, vapor pressure or water solubility. Testing will be conducted to evaluate these end points.

5.0 ENVIRONMENTAL FATE DATA

5.1.2 Biodegradability

5.1.2.2 Summary of Available Data

The Modified MITI Test (OECD Guideline 301C) was used to evaluate the biodegradability of 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio). After the 28-day test, the extent of biodegradation was 2%-5% based on oxygen uptake and HPLC determination respectively.

5.1.2.3 Data Assessment and Test Plan for Biodegradability

The available data are adequate and reliable. Additional biodegradation testing will not be conducted.

5.1.3 Hydrolysis

5.1.3.2 Summary of Available Data

No published or unpublished hydrolysis studies were located for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio).

5.1.3.3 Data Assessment and Test Plan for Hydrolysis

The potential for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio) to hydrolyze will be characterized in a technical discussion.

5.1.4 Photodegradation

5.1.4.2 Summary of Available Data

No published or unpublished photodegradation studies were located for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio).

5.1.4.3 Data Assessment and Test Plan for Photodegradation

The Atmospheric Oxidation Potential (AOP) of this substance will be characterized using the modeling program AOPWIN.

5.1.5 Fugacity Modeling

5.1.5.2 Summary of Available Data

No published or unpublished fugacity-based multimedia fate modeling data was located for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio).

5.1.5.3 Test Plan for Fugacity

The relative distribution of 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio) among environmental compartments will be evaluated using Level I Fugacity modeling.

Input data to run the EQC Level I model will require an additional computer model to estimate physical/chemical properties from a structure. The model used for this purpose will be EPIWIN, version 3.02¹, which was developed by the Syracuse Research Corporation. EPIWIN includes algorithms for estimating all physical and chemical properties needed for the EQC model.

5.2. ECOTOXICOLOGY DATA

5.2.1 Aquatic Ecotoxicity Testing

5.2.2.1 Summary of Available Data

The 96 hour LC₅₀ of 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio) determined in fathead minnows is > 1000 mg/L. The NOEL is 1000 mg/L.

5.2.2.2 Data Assessment and Test Plan for Acute Aquatic Ecotoxicity

The available aquatic toxicity data in fish are adequate and reliable. The HPV Challenge Program requires that acute aquatic ecotoxicity tests in fish, invertebrates, and algae be performed. Acute aquatic ecotoxicity testing in fish has been conducted. Additional aquatic toxicity testing in invertebrates and algae are proposed according to OECD Test Guidelines 202 and 201 respectively.

5.3 MAMMALIAN TOXICOLOGY DATA

5.3.1 Acute Mammalian Toxicity of 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio)

5.3.2.2 Summary of Available Data

Acute oral, dermal and inhalation toxicity studies are available for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio). The LD₅₀ in rats (oral) and rabbits (dermal) are >10 g/kg and

¹ Environmental Science Center- Syracuse Research Corporation- EPI for windows.

> 2 g/kg respectively. The inhalation LC₅₀ in rats is > 2.75 mg/L based on nominal concentration.

5.3.2.3 Data Assessment and Test Plan for Acute Mammalian Toxicity

The HPV Challenge Program requires that either an acute oral (preferable), dermal, or inhalation test be performed on, or bridged to, each HPV chemical. Adequate and reliable acute oral, dermal and inhalation toxicity tests were previously performed and were located for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio). Additional acute mammalian toxicity testing is not proposed.

5.3.3 Mutagenicity of 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio)

5.3.3.2 Summary of Mutagenicity Data

The HPV Challenge Program requires that a gene mutation test and a chromosome aberration test be performed on, or bridged to, each HPV chemical. A gene mutation and a chromosome aberration study have been conducted on 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio). Both studies were negative.

5.3.3.3 Data Assessment and Test Plan for Mutagenicity Toxicity

Adequate and reliable gene mutation and chromosome aberration studies were performed for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio). Additional mutagenicity testing will not be performed.

5.3.4 Repeated-dose, Reproductive and Developmental Toxicity of 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio)

5.3.4.2 Summary of Repeated-Dose Toxicity Data

No published or unpublished repeat dose, reproductive or developmental toxicity tests were located for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio).

5.3.4.3 Data Assessment and Test Plan for Repeated-dose Toxicity

The HPV Challenge Program requires repeated-dose toxicity and a reproductive/developmental toxicity study be performed or bridged to each HPV chemical. Testing of 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio) is proposed in the form of OECD Test Guideline 422: A Combined Repeated Dose Toxicity Study with a Reproduction/Developmental Toxicity Screening Test.

6.0 Summary

The testing proposed in Table 2 will complete the data acquisition for 1,3,4-thiadiazole, 2,5-bis(tert-nonyldithio) under the Environmental Protection Agency High Production Volume (HPV) Chemical Challenge Program.